2,2,8-Trimethyl-7-prop-2-ynoxychromene
94244-29-8 | DTXSID10241225

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 9.65e-11 cm3/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 1.50e-01

Confidence level: 8.51e-01

Nearest Neighbors from the Training Set

Image not found
alpha-Phellandrene
Measured: 3.13e-10
Predicted: 2.83e-10

Image not found
alpha-Humalene
Measured: 2.90e-10
Predicted: 2.87e-10

Image not found
2-Methyl-p-benzoquinone
Measured: 2.35e-11
Predicted: 2.15e-11

Image not found
(2E)-2-Hexenal
Measured: 4.40e-11
Predicted: 4.31e-11

Image not found
(3Z)-3-Hexenyl acetate
Measured: 7.80e-11
Predicted: 7.52e-11